Dichloroacetylene
7572-29-4 | DTXSID7020429

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 41.2 mmHg

Global applicability domain: Inside

Local applicability domain index: 5.12e-01

Confidence level: 5.43e-01

Nearest Neighbors from the Training Set

Image not found
Carbon tetrachloride
Measured: 115
Predicted: 63.5

Image not found
Dibromodifluoromethane
Measured: 39.0
Predicted: 781

Image not found
1-Chloro-2-propanol
Measured: 18.5
Predicted: 5.24

Image not found
Trimethylamine
Measured: 803
Predicted: 862

Image not found
Dimethyl sulfoxide
Measured: 2.10e-01
Predicted: 3.98e-01